Grazing Incidence and Co-planar Reflectivity Study of a Thin Thermal Oxide (SiO_2) Over Si(001)

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Beamline(s): **X22C**

Introduction: Thin layers of amorphous SiO_2 grown on Si substrates are widely used as gate oxides in semiconductor industry. One of the most remarkable properties of this material combination is the ideal (atomically smooth) match of the two substances, that enables the preparation of extremely thin oxide layers. However, the microscopic details of the structural gradient between the perfect silicon crystal and the amorphous SiO_2 layer are not clear. Models have been developed[1] that propose an ordered array of Si-O-Si bridges, resulting in a low strain energy of the interface.

Methods and Materials: Our approach to the problem of the structural gradient is depth-sensitive xray scattering under grazing incidence (GIXD) and exit conditions in order to determine the (amorphous) structure factor of SiO_2 near the interface and in the entire film. The samples under investigation have been prepared using high-temperature oxidation in an MBE-system, resulting in extremely smooth interfaces (rms roughness 3 Å). As a first step we investigated a smooth glass wafer in order to get a reference for the undistorted structure factor of SiO_2. The first five diffraction features of the amorphous structure factor are visible (not shown here) and will serve as a future reference for the thin film measurements. The z-axis geometry of X22C enabled us to set an incident angle as low as 2.5mrad (which is the critical angle for total external reflection for SiO_2 at the energy of 11000 eV used here) by rotating the diffractometer and performing detector scans in the vertical plane. The measurements have been performed in a protective He atmosphere.

Results: We now turn to the GIXD experiments for a 100 Å thick SiO_2 layer grown on Si(001). We performed radial scans through the Si(220) lying in the surface plane, covering a scattering depth of 100-200 Å. In addition to the sharp Si(220) Bragg reflection, a broad component is visible that is slightly off-center with respect to the Si reflection. The center of mass of the broad feature suggests a slightly (0.6%) higher lattice spacing and the width corresponds to about 150 Å correlation length. A closer look at the Si(220) reflection (inset of Figure 1) reveals a radial profile modified by a compressive strain in the Si. In order to shed light on this puzzling double peak feature we performed specular reflectivity measurements, yielding the electron density gradient perpendicular to the surface. Despite the low electron density contrast between Si and SiO_2 well defined thickness oscillations are visible. The inset of Figure 2 shows the intensity distribution multiplied by Q^4 in order to omit the Fresnel part of the reflectivity. This representation enhances the thickness oscillations for better recognition. A beating frequency on top of the $2\pi/100$Å frequency is obvious. This beating corresponds to a thickness of 12 Å, suggesting a second layer with different electron density in addition to the amorphous SiO_2.

Conclusions: To summarize, in a preliminary experiment we have demonstrated the feasability of GIXD on amorphous samples using a glass standard. We detected scattering signals from the Si/ SiO_2 interface that may be related to an ordered phase with 0.6% misfit. Furtheremore the Si surface is under compressive stress, most probable due to the thermal misfit to the SiO_2 layer resulting from the cooling process after preparation at 800C. The assumption of a modified transition layer at the Si/ SiO_2 interface[1] is supported by specular reflectivity measurements that show the presence of a second layer with modified density in addition to the SiO_2.

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References: [1]Yuhai Tu and J. Tersoff, Phys. Rev. Lett. **84**, 4393 (2000)

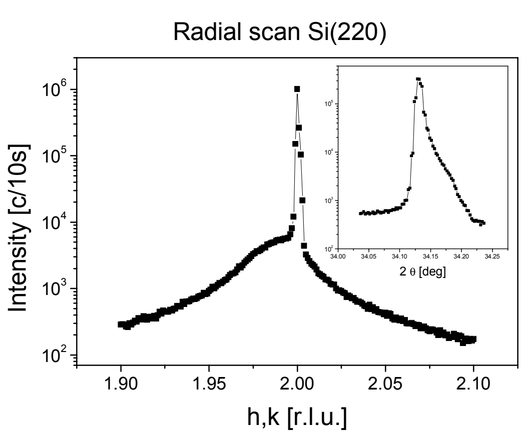

Figure 1. Inplane radial scan through the Si(220) reflection of a 100 Å SiO_2/Si(001) sample.

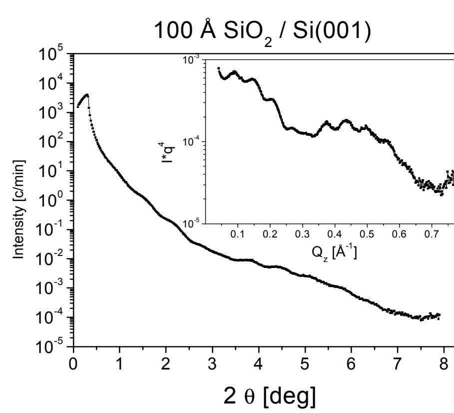

Figure 2. Specular reflectivity as a function of the detector angle of the same sample as in 1.